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PHYSICS

A METHOD OF CALCULATING GROUND-STATE PROPERTIES OF MANY PARTICLE SYSTEMS USING REDUCED DENSITY MATRICES

by

Claude Garrod and Jerome K. Percus

July 15, 1963

Institute of Mathematical Sciences

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ABSTRACT

The following problem is considered: Given an operator, $\Gamma(x_1,x_2|y_1,y_2)$, under what conditions can we be sure that there exists at least one quantum mechanical ensemble of N identical particles for which Γ represents the two-particle reduced density matrix. Fairly stringent necessary conditions are presented. In the classical limit these conditions are shown to be sufficient. Some simple applications are given.

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1. Introduction

For a system of bosons (fermions)* the usual form of the variational principle for the N-particle ground state of a hamiltonian operator, H, is that the N-particle ground-state energy, $E_o(N)$, is given by:

$$E_o(N) = \text{Min} \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \tag{1.1}$$

subject to the restriction that:

$$\langle \psi \mid (\hat{N} - N)^2 \mid \psi \rangle = 0 \quad , \tag{1.2}$$

where the trial states, $|\psi\rangle$, are chosen from a boson (fermion) Fock space, S_F, appropriate to the problem at hand. We may however somewhat trivially generalize the principle in a way which will prove convenient for our purposes. We may choose from the space of hermitian operators on S_F the set Ω of those operators which are non-negative. That is, the set of operators which when diagonalized take the form

$$\omega = \sum_n \lambda_n |\psi_n\rangle\langle\psi_n| \tag{1.3}$$

with all $\lambda_n \geq 0$.

Then the reader may easily verify that the N-particle ground-state energy is given by

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*Throughout this paper we shall treat the cases of bosons and fermions simultaneously. In order to do this we hereby introduce a variable σ which is +1 or −1 for bosons or fermions respectively.

(1.4) $$E_o(N) = \text{Min} \frac{\text{Trace } (H\omega)}{\text{Trace } \omega}$$

subject to the restrictions:

(1.4a) $$\text{Tr } ((\hat{N} - N)^2 \omega) = 0 \quad ,$$

(1.4b) $$\omega \in \Omega \quad .$$

If the hamiltonian operator H has a unique N-particle ground state then the operator which yields the minimum will be just the projection operator for that state

$$\omega_o = |\psi_o><\psi_o| \quad .$$

In practice the complexity of the N-particle states makes either scheme difficult if not impossible to carry out except for very special hamiltonians. There is another variational method, which we shall call the method of reduced density matrices, which seeks to exploit both the requirement of complete symmetry (antisymmetry) of the wave function with respect to coordinate interchange and the fact that the N-particle hamiltonian operators of real interest in physics are actually symmetric sums of one or two particle operators. This method, if correctly formulated, would avoid all reference to the complex N-particle wave functions. The initial formulation of the method is the following:

From each element ω of Ω we can construct a set of functions which will be called "reduced density matrices" as follows: Choose a complete set of boson (fermion) single-particle annihilation operators, a_n, $n = 1, 2, \ldots$. We then define the functions:

(1.5) $$\lambda = \text{Tr } \omega \quad ,$$

(1.6) $$\gamma(k \mid \ell) = \text{Tr } (a_k^+ a_\ell \omega) \quad ,$$

(1.7) $$\Gamma(k, \ell \mid m, n) = \text{Tr } (a_\ell^+ a_k^+ a_m a_n \omega) \quad .$$

If we are now given a hamiltonian operator of the form:

$$H = \sum T(k|\ell)\, a_k^+ a_\ell + \sum V(k,\ell|m,n)\, a_\ell^+ a_k^+ a_m a_n \tag{1.8}$$

then the N-particle ground-state energy is given by:

$$E_o(N) = \text{Min}\,[\lambda^{-1} \sum T(k|\ell)\gamma(k|\ell) + \lambda^{-1} \sum V(k,\ell|m,n)\Gamma(k,\ell|m,n)], \tag{1.9}$$

where we vary the functions γ and Γ subject to the restrictions:

(1.9a) (I) $\sum \gamma(k|k) = N\lambda$, $\sum \Gamma(k,\ell|k,\ell) = N(N-1)\lambda$.

(II) The set of functions $(\lambda, \gamma, \Gamma)$ is derivable from some operator in Ω by equations (1.5) to (1.7).

There are basically two ways of satisfying Condition II. One is to choose some class of operators in Ω and explicitly calculate the reduced density matrices obtained from them. This method will form the basis of some work to be published later. By using this method one does not at all avoid the difficulties involved in handling N-particle functions. Another method would be to find intrinsic necessary and sufficient conditions on the set of functions $(\lambda, \gamma, \Gamma)$ which would insure that Condition II was satisfied. It is the second method with which we shall concern ourselves in this paper. If the above-mentioned necessary and sufficient conditions could be found one could avoid all reference to the N-particle wave functions in determining the ground-state expectation values of any one- or two-particle operators. In what is probably the earliest reference to this problem J. von Neumann [1] shows that the necessary and sufficient condition that a reduced density matrix be derivable from an N-particle system is that it be a non-negative matrix. The reason for this very simple solution is that no restrictions are placed upon the N-particle wave functions with respect to particle interchange. Since that time a large number of workers [2-12] have either investigated this problem or made calculations taking account of Condition II in various approximate ways. The results to be reported in this paper are:

(1) A set of necessary and sufficient conditions which are not really intrinsic in that reference is made to a set of functions that cannot be explicitly written down.

(2) A set of intrinsic necessary conditions on the reduced density matrices is presented. Whether these conditions are sufficient to assure the satisfaction of Condition II is still an open question although it has been answered in the affirmative for some nontrivial cases.

2. Necessary and Sufficient Conditions

In order to derive our conditions we need first imbed the set of functions $(\lambda, \gamma, \Gamma)$ in a single Hilbert space. If we take: (1) a one-dimensional space U; (2) a Hilbert space of hermitian matrices of the form $h(k|\ell)$, call it S_h; and (3) a Hilbert space of hermitian double-index matrices of the form $H(k, \ell|m, n)$ which also satisfy the symmetry condition:

$$H(k, \ell|m, n) = \sigma H(k, \ell|n, m) \quad , \tag{2.1}$$

which we shall call S_H, then the set of functions $(\lambda, \gamma, \Gamma)$, taken as a single vector may be imbedded in the Hilbert space:

$$S = U \otimes S_h \otimes S_H \quad . \tag{2.2}$$

Once we have done this we may easily verify that the set of vectors in S which satisfy Condition II form a convex cone. A convex cone is a set of vectors with the property that if ξ_1 and ξ_2 are elements of the set and a_1 and a_2 are positive numbers then $a_1\xi_1 + a_2\xi_2$ is also an element of the set. We can now apply an established theorem on convex cones, a proof of which is given in Appendix A. A statement of the theorem is the following:

For each convex cone C in a Hilbert space we may define another convex cone $\widetilde{C}$, called the polar of C, as the set of all those vectors which have non-negative scalar products with every vector in C. The theorem is then that the polar of $\widetilde{C}$ is C. That is:

(2.3) $$C = \tilde{\tilde{C}} \quad .$$

Hence if we could describe the set $\tilde{C}$ we would have a method of determining whether a given vector was in the convex cone C made up of those reduced density matrices which satisfy Condition II. The fact that a vector $(F_o, F_1(k|\ell), F_2(k, \ell|m, n))$ is in $\tilde{C}$ means that for every set of reduced density matrices which satisfy Condition II:

(2.4) $$\lambda F_o + \sum \gamma(k|\ell) F_1(\ell|k) + \sum \Gamma(k, \ell|m, n) F_2(n, m|\ell, k) \geq 0 \quad .$$

By comparing it with equation (2.5) one can grasp the significance of the above equation immediately. If we look upon F_1 and F_2 as hamiltonian operators then equation (3.4) says that F_o must be larger than the negative of the lowest energy eigenvalue. At first sight it seems like a rather dismal situation in that one would have to solve a very wide class of ground-state energy problems in order to calculate the set $\tilde{C}$. However, if we consider different classes of hamiltonians for which we can calculate the ground-state energies we shall be able to derive various necessary if not sufficient conditions on proper reduced density matrices.

3. Necessary Conditions

Consider an operator of the form:

(3.1) $$A = C + f(k)a_k + g(k)a_k^+ + u(k_1, k_2)a_{k_1}a_{k_2} + v(k_1, k_2)a_{k_1}^+ a_{k_2}^+ + w(k_1, k_2)a_{k_1}^+ a_{k_2} \quad ,$$

where we have used the summation convention $f(k)a_k = \sum_k f(k)a_k$.

If we use the notation:

$$\langle \ldots \rangle = \mathrm{Tr}(\ldots \omega) \quad ,$$

where $\omega \in \Omega$ (i.e., a non-negative operator) then certainly:

(3.2) $$\langle A^{+}A \rangle \geq 0$$

The reader may easily verify that equation (3.2) may be written (again using the summation convention when multiplying matrix elements) in the form:

(3.3) $$[F]\,[D]\,[F] \geq 0$$

where F is a column vector whose elements are functions, i.e.:

(3.4) $$[F] = \begin{bmatrix} C \\ F(k) \\ g(k) \\ U(k_1,k_2) \\ V(k_1,k_2) \\ W(k_1,k_2) \end{bmatrix}$$

and:

$$D = \begin{bmatrix} \langle 1 \rangle & \langle a_k \rangle & \langle a_k^{+} \rangle & \langle a_{k_1} a_{k_2} \rangle & \langle a_{k_1}^{+} a_{k_2} \rangle & \langle a_{k_1}^{+} a_{k_2}^{+} \rangle \\ \langle a_\ell^{+} \rangle & \langle a_\ell^{+} a_k \rangle & \langle a_\ell^{+} a_k^{+} \rangle & \langle a_\ell^{+} a_{k_1} a_{k_2} \rangle & \langle a_\ell^{+} a_{k_1}^{+} a_{k_2} \rangle & \langle a_\ell^{+} a_{k_1}^{+} a_{k_2}^{+} \rangle \\ \langle a_\ell \rangle & \langle a_\ell a_k \rangle & \langle a_\ell a_k^{+} \rangle & \langle a_\ell a_{k_1} a_{k_2} \rangle & \langle a_\ell a_{k_1}^{+} a_{k_2} \rangle & \langle a_\ell a_{k_1}^{+} a_{k_2}^{+} \rangle \\ \langle a_{\ell_2}^{+} a_{\ell_1}^{+} \rangle & \langle a_{\ell_2}^{+} a_{\ell_1}^{+} a_k \rangle & \langle a_{\ell_2}^{+} a_{\ell_1}^{+} a_k^{+} \rangle & \langle a_{\ell_2}^{+} a_{\ell_1}^{+} a_{k_1} a_{k_2} \rangle & \langle a_{\ell_2}^{+} a_{\ell_1}^{+} a_{k_1}^{+} a_{k_2} \rangle & \langle a_{\ell_2}^{+} a_{\ell_1}^{+} a_{k_1}^{+} a_{k_2}^{+} \rangle \\ \langle a_{\ell_2}^{+} a_{\ell_1} \rangle & \langle a_{\ell_2}^{+} a_{\ell_1} a_k \rangle & \langle a_{\ell_2}^{+} a_{\ell_1} a_k^{+} \rangle & \langle a_{\ell_2}^{+} a_{\ell_1} a_{k_1} a_{k_2} \rangle & \langle a_{\ell_2}^{+} a_{\ell_1} a_{k_1}^{+} a_{k_2} \rangle & \langle a_{\ell_2}^{+} a_{\ell_1} a_{k_1}^{+} a_{k_2}^{+} \rangle \\ \langle a_{\ell_2} a_{\ell_1} \rangle & \langle a_{\ell_2} a_{\ell_1} a_k \rangle & \langle a_{\ell_2} a_{\ell_1} a_k^{+} \rangle & \langle a_{\ell_2} a_{\ell_1} a_{k_1} a_{k_2} \rangle & \langle a_{\ell_2} a_{\ell_1} a_{k_1}^{+} a_{k_2} \rangle & \langle a_{\ell_2} a_{\ell_1} a_{k_1}^{+} a_{k_2}^{+} \rangle \end{bmatrix} \tag{3.5}$$

Since no restrictions were placed upon the functions which are elements of F equation (3.3) clearly states that D is a non-negative operator. In analizing some of the consequences of equation (3.3) the first case we shall consider is that in which all elements of

D which contain an unequal number of creation and annihilation operators are zero. This does not correspond to the case in which the number of particles is fixed but rather to that in which the eigenstates of ω are states of fixed particle number. That is, the particle number dispersion is "classical". Then using our previous definitions for λ, γ, and Γ (equations 1.5, 1.6, and 1.7) the operator D reduces to:

$$D = \begin{bmatrix} \lambda & & & & \gamma(k_1|k_2) \\ & \gamma(\ell|k) & & & \\ & & g(\ell|k) & & \\ & & & \Gamma(\ell_1,\ell_2|k_1,k_2) & \\ \gamma(\ell_2|\ell_1) & & & G^{(1)}(\ell_1,\ell_2|k_1,k_2) & \\ & & & & G^{(2)}(\ell_1,\ell_2|k_1,k_2) \end{bmatrix} \tag{3.6}$$

where the functions g, $G^{(1)}$, and $G^{(2)}$ are related to the previously defined functions by:

$$(3.7)\quad g(\ell|k) = \lambda\delta_{\ell k} + \sigma\gamma(k|\ell)$$

$$(3.8)\quad G^{(1)}(\ell_1,\ell_2|k_1,k_2) = \delta_{k_1\ell_1}\gamma(\ell_2|k_2) + \sigma\Gamma(k_1,\ell_2|\ell_1,k_2)$$

$$(3.9)\quad G^{(2)}(\ell_1,\ell_2|k_1,k_2) = \Gamma(k_1,k_2|\ell_1,\ell_2) + \sigma\delta_{\ell_2k_2}\gamma(k_1|\ell_1) + \delta_{\ell_1k_2}\gamma(k_1|\ell_2) + \\ + \delta_{\ell_2k_1}\gamma(k_2|\ell_1) + \sigma\delta_{\ell_1k_1}\gamma(k_2|\ell_2) + \lambda\delta_{\ell_1k_1}\delta_{\ell_2k_2} + \sigma\lambda\delta_{\ell_1k_2}\delta_{\ell_2k_1}$$

The condition that the operator D be non-negative now decomposes into the four separate conditions that the diagonal

"elements" γ, g, Γ, and $G^{(2)}$ be non-negative operators and that the two-by-two matrix:

$$\tilde{G} = \begin{bmatrix} \lambda & \gamma \\ \gamma & G^{(1)} \end{bmatrix} \tag{3.10}$$

be a non-negative operator. The condition that the one-particle density matrix γ be non-negative is certainly well known. (see v. Neumann [1].). For a boson system the condition that g be non-negative is simply a weakened version of the condition on γ. This should be expected since the first condition is known to be sufficient to insure that a non-negative ω exists which would yield γ by equation (1.6). However, for a fermion system if we choose the representation in which γ is diagonal and if we take $\lambda = 1$, the conditions that both γ and g be non-negative yields the restriction on the eigenvalues of γ:

$$0 \leq \gamma(n|n) \leq 1 \quad . \tag{3.11}$$

That this condition is sufficient to insure that γ is derivable from some non-negative ω is proven in Appendix C. That Γ is non-negative is again a well known fact. For a boson system the fact that $G^{(2)}$ is non-negative is redundant, that is it can be derived from the non-negativity of λ, γ, and Γ. For a fermion system the non-negativity of $G^{(2)}$ yields an infinite sequence of inequalities relating matrix elements of γ and Γ. The first of these is simply the condition that the diagonal elements of $G^{(2)}$ are non-negative.

$$\Gamma(k,\ell|k,\ell) - \gamma(k|k) - \gamma(\ell|\ell) + 1 + \delta_{k\ell}(\gamma(k|\ell) + \gamma(\ell|k) - 1) \geq 0 \tag{3.12}$$

For $k = \ell$ since $\Gamma(k,k:k,k) = 0$ the above equation becomes an identity. For $k \neq \ell$ if we use, for the one- and two-particle distribution functions the symbols:

(3.13) $$\rho(k) = \gamma(k|k)$$

(3.14) $$\rho(k,\ell) = \Gamma(k,\ell|k,\ell)$$

we obtain:

(3.15) $$\rho(k,\ell) \geq \rho(k) + \rho(\ell) - 1 \quad .$$

This expresses the quite reasonable idea that if single-particle states k and ℓ are filled then there must be a pair in the pair state (k,ℓ). Restrictions of this type are important where the states k and ℓ are of low kinetic energy while the state (k,ℓ) is of large potential energy. If we ignore this type of restrictions when making a variational calculation on such a system using reduced density matrices then the set of reduced density matrices which yield the energy minimum will exhibit the phenomenon of "overcorrelation". That is, the two-particle correlation function will be inconsistent with the single particle distribution. What is probably the clearest example of overcorrelation is the following one due to J. E. Mayer. Consider N classical particles in a one dimensional periodic "box" of length L with distribution functions:

(3.16) $$\rho(X) = {}^{N}/_{L} \qquad 0 \leq X \leq L$$

(3.17a) $$\rho(X_1,X_2) = C \quad \text{if} \quad R \leq |X_1 - X_2| \leq L - R$$

(3.17b) $$\rho(X_1,X_2) = 0 \quad \text{otherwise,}$$

(3.17c) where: $C = \dfrac{N(N-1)}{L(L-2R)}$.

The above equations clearly describe a system of N particles with "hard cores" of diameter R. The distribution functions seem all right since they are always positive, symmetric, and:

$$(3.18) \qquad \rho(X) = \frac{1}{N-1} \int_0^L \rho(X,y)dy.$$

But if $R > {}^{L}/_{N}$ the above distribution functions describe the absurd situation of having N particles in a box in which they couldn't possibly fit. Certainly the above distribution functions could never be obtained from any N-particle system. We shall return to the Mayer example later in considering restrictions on the distribution functions for classical systems.

Returning to the analysis of the matrix $G^{(2)}$ for a fermion system, the fact that $G^{(2)}$ is non-negative implies that all its principle determinants are non-negative. That is, given any two sets of S indices, k_n, k'_n, $n = 1,2,..,S$. then the determinant:

$$(3.19) \qquad \begin{vmatrix} G(k_1,k'_1|k_1,k'_1)\ldots G(k_1,k'_1|k_S,k'_S) \\ \vdots \qquad\qquad\qquad \vdots \\ G(k_S,k'_S|k_1,k'_1)\ldots G(k_S,k'_S|k_S,k'_S) \end{vmatrix} \geq 0.$$

The most interesting restrictions are obtained from the non-negativity of $\tilde{G}$ where:

$$(3.10) \qquad \tilde{G} = \begin{bmatrix} \lambda & \gamma \\ \gamma^* & G^{(1)} \end{bmatrix}$$

Again choosing two sets of indices, k_n, k'_n, $n = 1,\ldots,S$, we form the test vector:

$$F = \begin{bmatrix} 1 \\ v(k,k') \end{bmatrix} \tag{3.20}$$

$$\text{where:} \quad v(k,k') = \sum_{n=1}^{S} X_n \delta(k-k_n)\delta(k'-k'_n) \tag{3.21}$$

and where the X_n are real parameters. Then, since G is non-negative:

$$(F,\tilde{G}F) = \lambda^2 + \lambda \sum_{n=1}^{S} X_n(\gamma(k_n|k'_n) + \gamma(k'_n|k_n)) + \tag{3.22}$$

$$+ \sum_{n,m}^{S} X_n X_m G^{(1)}(k_n,k'_n|k_m,k'_m) \geq 0$$

In order to eliminate the arbitrary parameters from condition (3.22) the reader is referred to Appendix B where it is proven that equation (3.22) is equivalent to the equations:

$$\text{Det } G^{(1)}(k_i,k'_i|k_j,k'_j) \geq 0 \tag{3.23}$$

and:

$$\text{Det } G^{(1)}(k_i,k'_i|k_j,k'_j) \geq \sum_{n=1}^{S} \bar{\gamma}(k_n|k'_n) \begin{vmatrix} G^{(1)}(1,1'|1,1')\cdots\bar{\gamma}(1|1')\cdots G^{(1)}(1,1'|S,S') \\ \\ \\ G^{(1)}(S,S'|1,1')\ldots\bar{\gamma}(S|S')..G^{(1)}(S,S'|S,S') \end{vmatrix} \tag{3.24}$$

where: $\overline{\gamma}(1|1') = \frac{1}{2}(\gamma(k_1|k_1') + \gamma(k_1'|k_1))$ etc. and λ has been taken equal to one.

We shall first try to interpret these conditions for bosons. In this case:

$$G(k,k'|\ell,\ell') = \delta_{k_\ell}\gamma(k'|\ell') + \Gamma(\ell,k'|k,\ell') \quad . \tag{3.25}$$

For $S = 1$ equation (3.23) is trivial but equation (3.24) yields:

$$\rho(k') + \rho(k,k') \geq (\overline{\gamma}(k|k'))^2 \tag{3.26}$$

The above seems to be a rather weak condition. One obvious consequence is that if: $\rho(k,k) = 0$ then: $0 \leq \rho(k) \leq 1$, or in words, if there is never a pair in the state (k,k) then the average nunber of particles in the state k cannot exceed one. For $S = 2$ equations (3.23) and (3.24) give:

$$(\rho(1')+\rho(1,1'))(\rho(2')+\rho(2,2')) - |\delta_{12}\gamma(1'|2') + \Gamma(2,1'|1,2')|^2 \geq \tag{3.27}$$

and:

$$\begin{aligned}(\rho(1')+\rho(1,1'))(\rho(2')+\rho(2,2')) - |\delta_{12}\gamma(1'|2') + \Gamma(2,1'|1,2')|^2 \geq \\ \geq (\overline{\gamma}(1|1'))^2(\rho(2')+\rho(2,2')) + (\overline{\gamma}(2|2'))^2(\rho(1')+\rho(1,1')) - \\ - 2\overline{\gamma}(1|1')\overline{\gamma}(2|2')(\delta_{12}\overline{\gamma}(1'|2') + \overline{\Gamma}(2,1'|1,2'))\end{aligned} \tag{3.28}$$

where: $\overline{\gamma} = \frac{1}{2}(\gamma+\gamma^*)$ and $\overline{\Gamma} = \frac{1}{2}(\Gamma + \Gamma^*)$.

If we choose $k_1 = k_1' \neq k_2 = k_2'$ then equations (3.27) and (3.28) may be written in the form:

(3.29) $\langle N_1^2\rangle\langle N_2^2\rangle \geq \langle N_1 N_2\rangle^2$

and:

(3.30) $\langle N_1^2\rangle\langle N_2^2\rangle - \langle N_1 N_2\rangle^2 \geq \langle(\langle N_1\rangle^2 N_2 - \langle N_2\rangle^2 N_1)^2\rangle$

where N_1 is the number operator for the state k_1. Certainly equation (3.29) simply states that we cannot occupy the pair state (k_1,k_2) with a large number of pairs without also increasing the occupation of the pair states (k_1,k_1) and (k_2,k_2). Equation (3.30) is a more detailed version of the same principle. Thus although we can only obtain weak bounds on the maximum occupation of a particular pair state (of the order of N^2) we can obtain strong relations among the occupation numbers of related pair states. The role which these restrictions play in forcing pairs to occupy states of higher kinetic energy in order to avoid pair states of high potential energy may be illustrated by applying equation (3.29) to a system which has only forward scattering repulsive interactions between particles in the same momentum state. The hamiltonian is:

(3.31) $H = \sum T_k a_k^+ a_k + \sum V_k a_k^+ a_k^+ a_k a_k$

Using the fact that, for an N-particle state: $N^{-1}\sum a_k^+ a_k |N\rangle = |N\rangle$ we may convert H to the form

(3.32) $H = \frac{1}{2N}\sum_{k,p}(\varepsilon_k+\varepsilon_p)a_k^+ a_k a_p^+ a_p + \sum_k V_k a_k^+ a_k a_k^+ a_k$

where: $\varepsilon_k = T_k - V_k$

Hence:

$$(3.33) \qquad \langle H \rangle = \frac{1}{2N} \sum_{k,p} (\varepsilon_k + \varepsilon_p) \langle N_k N_p \rangle + \sum V_k \langle N_k^2 \rangle$$

Since the energy of a pair in the state (k,p) is so much smaller than the energy of a pair in the state (k,k) the former states will have the maximum occupation consistent with:

$$(3.34) \qquad \langle N_k^2 \rangle \langle N_p^2 \rangle \geq \langle N_k N_p \rangle^2 .$$

We may take as our variables:

$$(3.35) \qquad U_k = \langle N_k^2 \rangle^{1/2}$$

If we assume the equality sign holds in equation (3.34) then:

$$(3.36) \qquad \sum_{k\ p} \langle N_k N_p \rangle = \left(\sum_k U_k\right)^2 = N^2$$

$$(3.37) \qquad \text{or:} \quad \sum_k U_k = N$$

Introducing a Lagrange parameter, α, by:

$$(3.38) \qquad \langle H_\alpha \rangle = \langle H \rangle - \alpha \sum U_k = \sum (\varepsilon_k - \alpha) U_k + \sum V_k U_k^2 \quad .$$

The minimum of $\langle H_\alpha \rangle$ is given by the equations:

$$(3.39) \qquad \frac{\partial \langle H_\alpha \rangle}{\partial U_k} = \varepsilon_k - \alpha + 2 V_k U_k = 0$$

$$(3.40) \qquad \text{that is:} \quad U_k = \frac{\alpha - \varepsilon_k}{2 V_k} \quad \text{for} \quad |k| \leq \mathcal{K}$$

and

(3.41) $U_k = 0$ for $|k| > K$

(3.42) where K is given by: $\alpha = \varepsilon_K$.

The normalization condition is now:

$$(3.43) \qquad \sum_{|k|<K} \frac{\varepsilon_K - \varepsilon_k}{2V_k} = N \quad .$$

or, for three dimensional particles in a box of volume Ω, if we approximate the sum by an integral:

$$(3.44) \qquad \frac{\Omega}{(2\pi)^2} \int_0^K \frac{\varepsilon_K - \varepsilon_k}{V_k} k^2 dk = N$$

or:

$$(3.45) \qquad \int_0^K \frac{\varepsilon_K - \varepsilon_k}{V_k} k^2 dk = (2\pi)^2 \rho$$

where ρ is the density of the system. The energy of the ground state is given by:

$$(3.46) \qquad E = \sum \varepsilon_k U_k + \sum V_k U_k^2$$

$$= \frac{1}{4} \sum_{|k|<K} \frac{\varepsilon_K^2 - \varepsilon_k^2}{V_k}$$

or again for a large three dimensional system:

$$(3.47) \qquad \frac{E}{} = \frac{1}{8\pi^2} \int_0^K \frac{\varepsilon_K^2 - \varepsilon_k^2}{V_k} k^2 dk.$$

One favorable characteristic of these results is immediately apparent. Since equation (3.45) gives $\mathcal{K}$ as a function of ρ we are assured that in (3.47) the total energy E will be proportional to the volume for fixed density. If we consider the case in which V_k is a positive constant, V_o, we find that the momentum distribution is given by:

$$(3.48) \qquad \langle N_k \rangle = C(\mathcal{K}^2 - k^2) \quad k^2 \leq \mathcal{K}^2$$

where: $C = \dfrac{\hbar^2}{4mV_o}$

and $\mathcal{K}$ is determined by:

$$(3.49) \qquad \mathcal{K}^5 = \frac{60\pi^2 mV_o\rho}{\hbar^2}$$

Let us now consider equations (3.23) and (3.24) for the case of fermions. Then:

$$(3.50) \qquad G^{(1)}(1,1'|2,2') = \delta_{12}\gamma(1'|2') - \Gamma(2,1'|1,2').$$

For $S = 1$ the equations take the form:

$$(3.51) \qquad \rho(k') \geq \rho(k,k')$$

and:

$$(3.52) \qquad \rho(k') - \rho(k,k') \geq (\bar{\gamma}(k|k'))^2 \quad .$$

Equation (3.51) is a direct consequence of the Pauli principle; since there can never be more than one particle in the state k then the conditional density of the state k assuming k' is filled must be less than one, or:

$$\frac{\rho(k,k')}{\rho(k')} \leq 1 \tag{3.53}$$

For $S = 2$ equations (3.23) and (3.24) are:

$$(\rho(1')-\rho(1,1'))(\rho(2')-\rho(2,2'))-|\delta_{12}\gamma(1'|2')-\Gamma(2,1'|1,2')|^2 \geq 0 \tag{3.54}$$

and:

$$\begin{aligned}(\rho(1')-\rho(1,1'))(\rho(2')-\rho(2,2'))-|\delta_{12}\gamma(1'12')-\Gamma(2,1'|1,2')|^2 \geq \\ \geq (\bar{\gamma}(1|1'))^2(\rho(2')-\rho(2,2'))+(\bar{\gamma}(2|2'))^2(\rho(1')-\rho(1,1')) - \\ - 2\bar{\gamma}(1|1')\bar{\gamma}(2|2')(\delta_{12}\bar{\gamma}(1'|2')-\bar{\Gamma}(2,1'|1,2'))\end{aligned} \tag{3.55}$$

In order to illustrate the content of these equations we shall apply (3.54) to the problem of obtaining an upper bound on the average value in an N-particle system of a given two-particle state projection operator. We shall assume that our system contains a finite number of single-particle states. This restriction can be relaxed at the end. It is not difficult to verify [12] that the destruction operator for any such two-particle state may be written in some representation in the form:

$$F = \sum_{n=-S}^{S} \lambda_n a_n a_{-n}, \quad \lambda_{-n} = -\lambda_n. \tag{3.56}$$

Hence the quantity we want to investigate is:

$$\Lambda = \langle F^\dagger F \rangle = \sum_{\substack{n,m \\ =-S}}^{S} \lambda_n \Gamma(n,-n|m,-m)\lambda_m \tag{3.57}$$

Now equation (3.54) is equivalent to (in fact was derived from) the equation; true for any values of x_1 and x_2:

$$(3.58)\quad x_1^2 G^{(1)}(1,1'|1,1')+x_2^2 G^{(1)}(2,2'|2,2') \geq \pm 2x_1 x_2 G^{(1)}(1,1'|2,2')$$

We now choose: $x_1 = \lambda_n$, $x_2 = \lambda_m$

and: $k_1 = -m$, $k_1' = -n$, $k_2 = n$, $k_2' = m$.

Then (3.58) can be written:

$$(3.59)\quad \lambda_n^2 \langle a_{-n}^+ a_{-m} a_{-m}^+ a_{-n} \rangle + \lambda_m^2 \langle a_m^+ a_n a_n^+ a_m \rangle \geq \pm 2\lambda_n \lambda_m \langle a_{-n}^+ a_{-m} a_n^+ a_m \rangle$$

Summing over n and m and using the commutation relations we obtain:

$$\sum_{n,m} \lambda_n^2 (1+\delta_{nm}) \langle N_{-n} \rangle - \langle N_{-n} N_{-m} \rangle +$$

$$+ \sum_{n,m} \lambda_m^2 (1+\delta_{nm}) \langle N_m \rangle - \langle N_m N_n \rangle \geq \pm 2 \sum_{n,m} \lambda_n \lambda_m (\delta_{n+m} \gamma(-n|m) +$$

$$+ \Gamma(n,-n|m,-m)) \qquad (3.60)$$

Using the facts that:

$$\sum_m 1 = 2S \quad \text{and:} \quad \sum_m \langle N_{-n} N_{-m} \rangle = N \langle N_{-n} \rangle,$$

we obtain:

$$(3.61)\quad (2S-N+2) \sum_n \lambda_n^2 \langle N \rangle \geq \pm \sum_{n,m} \lambda_n \lambda_m \Gamma(n,-n|m,-m)$$

It can be shown [12, Appendix A] that the maximum value of Λ is obtained in the case: $\lambda_1 = \lambda_2 = \ldots = \lambda_S$. Then (3.61) gives, for a normalized state:

$$(3.62)\qquad \Lambda \leq \pm N\left(\frac{2S-N+2}{2S}\right)$$

The same bound was obtained by C. N. Yang[12]. However, since our object is to develop a method of making calculations on N-particle systems without making reference to the N-particle wave functions it would be preferable if we could derive the above bound without using the fact, derived only from a detailed analysis of the wave function, that the maximum of Λ is obtained for the case $\lambda_1, = \lambda_2 = \ldots = \lambda_S$. Such a derivation is carried out in Appendix D for the case of a system with an infinite number of states.

4. General Case

We have looked at some of the consequences of imposing our necessary restrictions on the set of reduced density matrices for an N-particle system for the case in which all non-particle-conserving operators had vanishing average values. We must now return to the general case. Looking at the matrix D of equation (3.5) we see that the simplest non-trivial principle sub-matrix of D is:

$$d = \begin{bmatrix} \lambda & \nu(k) \\ \nu^*(\ell) & \gamma(\ell|k) \end{bmatrix} \tag{4.1}$$

where: $$\nu(k) \doteq \langle a_k \rangle . \tag{4.2}$$

Since the non-negativity of γ is necessary but not sufficient to insure that d be non-negative we see that not all non-negative single-particle density matrices describe real N-particle

systems with non-vanishing dispersion. Let us apply the condition that d be non-negative to the simple problem of a free field with external sources. The hamiltonian is:

$$(4.3) \qquad H = \sum (T_k a_k^+ a_k + \tfrac{1}{2} V_k (a_k^+ + a_k))$$

Assuming the field is real the energy is then:

$$(4.4) \qquad E = \sum (T_k \rho(k) + V_k \nu(k)) \ .$$

But the simplest possible condition on the principle sub-determinants of d, arising from the non-negativity of d is; (with $\lambda = 1$):

$$(4.5) \qquad \rho_k \geq (\nu(k))^2$$

For positive V_k the lowest value of E consistent with the inequality (4.5) will be obtained when:

$$(4.6) \qquad \nu(k) = - \sqrt{\rho(k)} \ .$$

The energy in this case is:

$$(4.7) \qquad E = \sum (T_k \rho(k) - V_k \sqrt{\rho(k)})$$

Defining: $U_k = \sqrt{\rho(k)}$ and setting the variation of E with respect to U_k equal to zero we obtain:

$$(4.8) \qquad U_k = \frac{V_k}{2T_k}$$

If the particles are bosons so there is no restriction on the value of U_k then the ground state energy we obtain is:

$$(4.9) \qquad E_o = -\frac{1}{4}\sum \frac{V_k^2}{T_k}$$

It is easy to confirm that this is the true ground state energy since the hamiltonian may be diagnolized by the canonical transformation:

$$(4.10) \qquad b_K = a_K - \frac{V_K}{2T_K}$$

In case the particles are fermions one must take into account the additional restriction:

$$(4.11) \qquad 0 \leq \rho_k \leq 1 \ .$$

If U_k as defined in (4.8) is smaller than one for all k then we have no difficulty with the exclusion principle and we obtain the same result as we did for bosons. If not, then whenever equation (4.8) would give U_K greater than one the exclusion principle limits the density to unity.

Moving now to the next order of complexity, we consider the following non-negative sub-matrix of D:

$$(4.12) \qquad d = \begin{bmatrix} 1 & \nu(\ell) & \nu^*(\ell) \\ \nu^*(k) & \gamma(k|\ell) & \nu^*(\ell,k) \\ \nu(k) & \nu(k,\ell) & g(k,\ell) \end{bmatrix}$$

$$(4.13) \qquad \text{where:} \quad \nu(k,\ell) = \langle a_k a_\ell \rangle$$

$$(4.14) \qquad \text{and:} \quad g(k,\ell) = \delta_{k\ell} + \sigma\gamma(\ell|k)$$

Again let us illustrate the use of the restrictions obtained from

demanding that d be non-negative by applying them to a well known problem; namely calculating the ground state properties of the reduced Bogoliubov hamiltonian. This is the hamiltonian obtained if one treats the zero-momentum creation and annihilation operators for a boson system as scalars. It is:

$$(4.15) \qquad H = \sum (T_k a_k^+ a_k + \frac{1}{2} V_k (a_k a_{-k} + a_k^+ a_{-k}^+))$$

For this hamiltonian the energy is given in terms of the functions ρ and ν by:

$$(4.16) \qquad E = \sum (T_k \rho_k + V_k \nu(k,-k))$$

where we have assumed: $\nu^* = \nu$. If the matrix d is non-negative then:

$$(4.17) \qquad \rho(k)(1+\rho(-k)) \geq (\nu(k,-k))^2$$

Since the hamiltonian is symmetric with respect to the transformation, $k \longrightarrow -k$, we may assume that $\rho(k) = \rho(-k)$. If V_k is positive the choice of $\nu(k,-k)$ which minimizes the energy while still satisfying the inequality (4.17) is clearly:

$$(4.18) \qquad \nu(k,-k) = - \sqrt{\rho(k)(1+\rho(k))}$$

If V_k is negative we need only reverse the sign in (4.18). Hence we may write the ground state energy entirely in terms of ρ.

$$(4.19) \qquad E = \sum (T_k \rho(k) - |V_k| \sqrt{\rho(k)(1+\rho(k))})$$

Defining a new function $\mu(k)$ by:

$$\mu(k) = \rho(k) + {}^1/_2 \tag{4.20}$$

we obtain:

$$E = \sum (T_k(\mu(k) - {}^1/_2) - |V_k|\sqrt{\mu^2(k) - {}^1/_4}\ ) \tag{4.21}$$

The variational equation with respect to $\mu(k)$ is:

$$\frac{\partial E}{\partial \mu(k)} = T_k - |V_k| \frac{\mu(k)}{\sqrt{\mu^2(k) - {}^1/_4}} = 0 \tag{4.22}$$

or

$$\mu(k) = \frac{T_k}{2\sqrt{T_k^2 - V_k^2}} \quad . \tag{4.23}$$

Using this value in equation (4.21) we obtain for the ground state energy:

$$E = -\frac{1}{2} \sum (T_k - \sqrt{T_k^2 - V_k^2}\ )$$

which is exactly the result derived by Bogoliubov using his canonical transformation method. The larger determinants of D involve matrix elements such as $\langle a_k a_\ell a_m \rangle$ which do not commonly occur in physical problems therefore we shall turn our attention instead to classical systems where we shall investigate the properties of the reduced density functions, $\rho(x)$ and $\rho(x_1, x_2)$.

5. Classical Systems

Since a classical system may be considered as a special case of a quantum mechanical system in which all density operators are diagnolized we may derive restrictions on classical reduced

density functions by considering those restrictions which involve only the diagonal elements, $\rho(x)$ and $\rho(x_1,x_2)$. The condition that γ and Γ are non-negative imply only the well known conditions that $\rho(x)$ and $\rho(x_1,x_2)$ be non-negative functions. The only remaining restriction which is not redundant is that $\tilde{G}$ is a non-negative operator. That is, given any function $F(x_1,x_2)$ and any constant, C:

$$C^2 + 2C\int F(x_1,x_2)\gamma(x_1|x_2)dx_1dx_2 + \\ + \int F(x_1,x_2)G^{(1)}(x_1,x_2|y_1,y_2)F(y_1,y_2)dx_1dx_2dy_1dy_2 \geq 0. \tag{5.1}$$

If we define:

$$G(x_1,x_2|y_1,y_2) = G^{(1)}(x_1,x_2|y_1,y_2) - \gamma(x_1|x_2)\gamma(y_1|y_2) \tag{5.2}$$

we see:

$$(C+\int F(x_1,x_2)\gamma(x_1|x_2)dx_1dx_2)^2 + \int F(x_1,x_2)G(x_1,x_2|y_1,y_2)F(y_1,y_2)x \\ xdx_1dx_2dy_1dy_2 \geq 0 \tag{5.3}$$

For a given function F the value of C which minimizes the above and hence yields the strongest restriction is that which makes the first term vanish. Thus we see that G is a non-negative matrix. From this, if we use the test function:

$$F(x_1,x_2) = \delta(x_1-x_2)F(x_1) \tag{5.4}$$

we obtain the following restriction on the reduced density functions:

$$(5.5) \qquad F(x)(\rho(x,y) + \delta(x-y)\rho(y) - \rho(x)\rho(y))F(y)dxdy \geq 0.$$

But this is just the condition that the operator:

$$(5.6) \qquad K(x,y) = \rho(x,y) + \delta(x-y)\rho(y) - \rho(x)\rho(y)$$

be non-negative. If $\rho(x,y)$ depends only upon $r = |x-y|$ then the eigenvalues of K are the fourier coefficients. The condition on K is then:

$$(5.7) \qquad \rho_o \int_{-\infty}^{\infty} g(r)\cos kr\,dr \leq 1 \quad \text{for all} \quad k$$

$$(5.8) \qquad \text{where:} \quad \rho(x,y) = \rho_o^2(1-g(r))$$

$$(5.9) \qquad \text{and:} \quad \rho_o = {}^{N}/_{L}$$

If we now reconsider the distribution, presented in Section 3, in which the two-particle density is constant except for a hard-core of diameter d we see that equation (5.7) demands that:

$$(5.10) \qquad d \leq \frac{L}{2N} \quad .$$

Thus not only the obviously absurd situation is omitted but the uniformity of the density demands that the excluded volume be no greater than half the total volume.

With an eye to eventually answering the question of whether these conditions (equation 5.5) are sufficient in the classical case to guarantee realizability of the one-and two-particle distributions let us investigate this problem from a slightly different point of view. Any symmetric N-particle distribution

may be written as a sum with positive coefficients of distributions which each describe the situation of having N particles at definite positions, $\lambda_1,\ldots,\lambda_N$. That is, take the set $C(\Lambda)$ of all distinct sets of N points, $\Lambda = (\lambda_1,\ldots,\lambda_N)$, then the N-particle distribution may be written:

$$(5.11)\qquad \rho(x_1,\ldots,x_N) = \sum_{C(\Lambda)} \alpha_\Lambda \sum_{\text{perm.}} \delta(x_1-\lambda_1)x\ldots x\delta(x_N-\lambda_N)$$

where the second sum is over all the permutations of the x_i and:

$$(5.12)\qquad \sum_{C(\Lambda)} \alpha_\Lambda = 1 \ .$$

One can now calculate the one- and two-particle distributions in terms of these "Λ" distributions:

$$(5.13)\qquad \rho(x) = \sum_{C} \alpha_\Lambda \sum_{i} \delta(x-\lambda_i)$$

$$(5.14)\qquad \rho(x,y) = \sum_{C} \alpha_\Lambda \left[\sum_{i,j} \delta(x-\lambda_i)\delta(y-\lambda_j) - \delta(x-y) \sum_{i} \delta(y-\lambda_i)\right]$$

We are now in a position to exhibit $K(x,y)$ explicitly as a sum, with positive coefficients, of manifestly non-negative operators. Using equations (5.12), (5.13), and (5.14) it is not difficult to verify that:

$$(5.15)\qquad K(x,y) = \sum_{C(\Lambda),C(\Lambda')} \alpha_\Lambda\alpha_{\Lambda'} \sum_{i,j} (\delta(x-\lambda_i)-\delta(x-\lambda'_i))(\delta(y-\lambda_i)-\delta(y-\lambda'_j)) \ .$$

We shall now give an argument to indicate that under some quite non-restrictive assumptions the condition given by equation (5.5) is sufficient to insure the realizability of the pair distribution function. We first assume that our variable, x, is discrete. Physically one could make the lattice spacing arbitrarily fine. We now make the additional assumption that the probability of finding two particles at the same lattice point is zero; that is, $\rho(n,n) = 0$. Rather than work with the two-particle distribution itself we introduce an associated matrix:

$$\tilde{K}(n,m) = \frac{\rho(n,m) + \delta_{nm}\rho(m)}{N} \quad . \tag{5.16}$$

Then the necessary conditions we have obtained describe a convex set of all those matrices which have the following properties:

(I) $\tilde{K}(n,m)$ is a non-negative matrix.

(II) $\tilde{K}(n,m) = \tilde{K}(m,n)$.

(III) $\sum_{n,m} \tilde{K}(n,m) = N$

(IV) $\tilde{K}(n,m) \geq 0$ for all n and m.

(v) $N\tilde{K}(n,n) = \sum_{m} \tilde{K}(n,m)$ for all n.

If, given some function $v(n,m)$, we now want to find the minimum of:

$$\bar{v} = \sum_{n,m} \tilde{K}(n,m)v(n,m) \tag{5.17}$$

within this set then we may do so by taking account of conditions I, II, III, and IV explicitly while satisfying the remaining

condition by the use of Lagrange parameters. The set of matrices which satisfy the first three conditions is the convex set generated by the projection operators; by which we mean that given any matrix $A(n,m)$ satisfying I, II, and III it is possible to find vectors, $a_S(n)$ $(S=1,2,...)$ and positive constants C_S such that:

$$A(n,m) = N\sum_S C_S a_S(n) a_S(m) \tag{5.18}$$

$$\text{and:} \quad \sum_S C_S = 1 \quad . \tag{5.19}$$

The most obvious example of such a set of vectors and constants is just the set of eigenvectors and eigenvalues however there generally exist other sets which may not utilize orthogonal vectors and may in general require more vectors than there are rows in the matrix. If we now impose condition IV we see that the only projection operators which survive are those for positive vectors (vectors with all non-negative components). The weakest point in our argument is the following: We conjecture that the set of matrices which satisfy conditions I through IV is generated by the projection operators for positive vectors. In Appendix E the conjecture is proven for two-by-two and three-by-three matrices. Then we may satisfy conditions I through IV explicitly by assuming that $\tilde{K}$ may be written:

$$\tilde{K}(n,m) = N \sum_S C_S F_S(n) F_S(m) \tag{5.20}$$

$$\text{where:} \quad C_S \geq 0, \quad F_S(n) \geq 0 \tag{5.21}$$

(5.22) and: $\sum_S C_S = \sum_n F_S^2(n) = 1.$

If our matrices have p rows and columns we can now satisfy condition V by introducing p Lagrange parameters, β_n (n=1,...,p) in the following way for the matrix v(n,m) whose minimum we want to obtain we replace a matrix $v_\beta(n,m)$ given by:

(5.23) $v_\beta(n,m) = v(n,m) + \sum_{k=1}^{p} \beta_k(N\delta_{nk}\delta_{mk} - \frac{1}{2}\delta_{nk} - \frac{1}{2}\delta_{mk}).$

For each set of β_n we now consider the minimum of:

(5.24) $\bar{v}_\beta = N \sum_{S,n,m} C_S F_S(n) v_\beta(n,m) F_S(m)$.

That minimum will in fact be given by the positive vector, call it F_β, which minimizes $(F, v_\beta F)$. We again weaken the argument by ignoring any difficulties that might arise if this vector is not unique. Then:

(5.25) $\text{Min } \bar{v}_\beta = N \sum F_\beta(n) v_\beta(n,m) F_\beta(m)$.

We now find the value of β_n for which condition V is satisfied by $K_\beta(n,m) = NF_\beta(n)F_\beta(m)$. This then yields the matrix K_β which minimizes v under the restrictions I through V. Let us now look at the minimizing matrix more carefully. Condition V states that:

(5.26) $NF_\beta^2(n) = F_\rho(n) \sum_m F_\beta(m)$.

This means that either $F_\beta(n)$ is zero or:

$$F_\beta(n) = \frac{1}{N} \sum_m F_\beta(m) = \frac{\text{const.}}{N} \quad .$$

The reader may easily convince himself that when we couple this with the condition that:

$$\sum_n F_\beta^2(n) = 1$$

the only possibility is that $F_\beta(n)$ be a vector with exactly N non-zero elements each of which is equal to $N^{-1/2}$. Hence the minimizing matrix K_β is clearly derivable from an N-particle system since it is in particular derivable from one of the "$\wedge$" distributions. Thus for any matrix $v(n,m)$ the minimum value we obtain in the convex set of matrices satisfying conditions I through V is the same as the minimum we would obtain by using that set of matrices which could be derived from N-particle distributions. But this was just the condition which we saw in Section 3 was necessary and sufficient for the two sets of matrices to be identical. Therefore any matrix satisfying conditions I through V may be derived from some N-particle distribution. The associated matrix $\rho(n,m)$ may also be appropriately derived from some N-particle distribution. It should be mentioned that the somewhat shaky sufficiency argument which has been presented for the "classical" case is applicable to the diagonal elements of Γ in any representation.

Appendix A

Let $\mathcal{K}$ be a closed convex cone in a Hilbert space, S. i.e.:

$x_1 \varepsilon \mathcal{K}$ and $x_2 \varepsilon \mathcal{K}$ implies

$ax_1 + bx_2 \varepsilon \mathcal{K}$ $\quad a, b \geq 0$.

Consider a set $\tilde{\mathcal{K}}$, defined as follows:

(A.1) $\quad \tilde{\mathcal{K}} = y:(x,y) \leq 0$ for every $x \varepsilon \mathcal{K}$

Lemma: $\tilde{\mathcal{K}}$ is a closed convex cone.

Proof: (A.2) $\quad (ay_1 + by_2, x) = a(y_1,x) + b(y_2,x) \leq 0$

Suppose $\quad y_n \rightarrow y_\infty$.

Then $\quad (y_n,x) \rightarrow (y_\infty,x)$.

But every $\quad (y_n,x) \leq 0$.

Hence $\quad (y_\infty,x) \leq 0$.

Theorem: $\quad \tilde{\tilde{\mathcal{K}}} = \mathcal{K}$

Proof: (A.3) $\quad$ (Part I) $\quad \mathcal{K} \subset \tilde{\tilde{\mathcal{K}}}$

Suppose $X \varepsilon \mathcal{K}$, then for every $y \varepsilon \mathcal{K}$ $(x,y) \leq 0$. Hence $\mathcal{K} \subset \tilde{\tilde{\mathcal{K}}}$.

(A.4) $\quad$ (Part II) $\quad \tilde{\tilde{\mathcal{K}}} \subset \mathcal{K}$.

Assume (A.4) is false. Then we may find at least one element, a, such that:

(A.5) $\quad a \notin \mathcal{K}$

(A.6) $\quad (a,y) \leq 0$ for all $y \varepsilon \tilde{\mathcal{K}}$

Let: $\quad r = g.\ell.b.|a-x|$ for all $x \varepsilon \mathcal{K}$

Since $\mathcal{K}$ is closed, $r > 0$.

Consider a sequence, $r_n > r$, such that $r_n \to r$. Construct the sequence of spheres of radius r_n about a.

$$\mathcal{S}_n = \{u : |u-a| \leq r_n\}$$

$\mathcal{S}_n$ is a closed convex set. Let I_n be the intersection of $\mathcal{S}_n$ and $\mathcal{K}$. Then I_n is a closed convex set.

Consider two sequences,

$$v_n \in I_n \quad \text{and} \quad v_n' \in I_n$$

Then: $r \leq |v_n - a| \leq r_n$.

Hence: $|v_n - a| \to r$.

Similarly: $|v_n' - a| \to r$.

We construct the midpoint of v_n and v_n'.

$$\overline{v}_n = \tfrac{1}{2} v_n + \tfrac{1}{2} v_n' \in I_n$$

Then:

$$(a-\overline{v}_n, a-\overline{v}_n) = (a,a) - (a,\overline{v}_n) - (\overline{v}_n,a) + (\overline{v}_n,\overline{v}_n)$$

$$= (a,a) - \tfrac{1}{2}(a,v_n) - \tfrac{1}{2}(a,v_n') - \tfrac{1}{2}(v_n,a) - \tfrac{1}{2}(v_n',a) + \tfrac{1}{4}(v_n,v_n)$$

$$+ \tfrac{1}{4}(v_n,v_n') + \tfrac{1}{4}(v_n',v_n) + \tfrac{1}{4}(v_n',v_n')$$

Hence:

$$(a-\overline{v}_n, a-\overline{v}_n) - \tfrac{1}{2}(a-v_n, a-v_n) - \tfrac{1}{2}(a-v_n', a-v_n') = -\tfrac{1}{4}(v_n-v_n', v_n-v_n')$$

But: $(a-\overline{v}_n, a-\overline{v}_n) \to (a-v_n, a-v_n) \to (a-v_n', a-v_n') \to r^2$

Therefore: $|v_n - v_n'| \to 0$

Hence the intersection, I_n, converges to a point. Since the convex cone $\mathcal{K}$ is closed: $I_n \rightarrow x_o$ where $x_o \in \mathcal{K}$.

We shall prove the following two statements which will then contradict our hypothesis:

(A) $a - x_o \in \mathcal{K}$ (B) $(a-x_o,a) > 0$

(A) Let $x \in \mathcal{K}$. Then $x_o + \varepsilon x \in \mathcal{K}$ $\varepsilon \geq 0$

Hence: $(a-x_o-\varepsilon x, a-x_o-\varepsilon x) > (a-x_o,a-x_o)$

$- (a-x_o,x) + \frac{\varepsilon}{2}(x,x) > 0$ for all $\varepsilon \geq 0$

Letting $\varepsilon \rightarrow 0$ we see:

$$(a-x_o,x) \leq 0$$

(B) $$\frac{d}{d\varepsilon} (a-(1+\varepsilon)x_o, a-(1+\varepsilon)x_o)\Big|_{\varepsilon = 0} = 0$$

Therefore: $(a-x_o,x_o) = 0$

But: $(a-x_o,a-x_o) = 2(a-x_o,a) > 0$.

Appendix B

Given a quadratic inequality:

$$(B.1)\quad Q(x_1,..,x_N) = \sum_{n,m}^{N} a_{nm}x_n x_m + 2\sum_{n}^{N} b_n x_n + C \geq 0 \quad \text{for all} \quad x_n,$$

one can immediately see that:

$$C \geq 0$$

and a_{nm} is a non-negative matrix. Also the vector b_n must be orthogonal to the null space of a_{nm}. If we assume that a_{nm} is a positive definite matrix then Q has a single minimum, $Q(x_1^o,...,x_N^o)$, and condition (B.1) is equivalent to the condition:

$$(B.2)\qquad Q(x_1^o,..,x_N^o) \geq 0$$

The values of x_n^o are the solution to the linear equations:

$$(B.3)\qquad \sum_m a_{nm}x_m + b_n = 0. \qquad n=1,...,N\ .$$

Hence:

$$(B.4)\qquad Q(x_1^o,...,x_N^o) = \sum b_n x_n^o + C \geq 0\ .$$

Using the explicit solutions:

$$(B.5)\qquad x_n^o = -\ \frac{\begin{vmatrix} a_{11}\cdots b_1 \cdots a_{1N} \\ a_{N1}\cdots b_N \cdots a_{NN} \end{vmatrix}}{|a_{ij}|}$$

we obtain the following condition which no longer involves the variables x_n:

$$(B.6) \qquad C|a_{ij}| \geq \sum_{n}^{N} b_n \begin{vmatrix} a_{11} \cdots b_1 \cdots a_{1N} \\ \vdots \qquad\qquad \vdots \\ a_{N1} \cdots b_N \cdots a_{NN} \end{vmatrix} .$$

Appendix C

Using the method of Section 2 applied to the set (λ,γ) it is easy to show that the necessary and sufficient conditions for the derivability of γ from some non-negative ω are that:

$$(C.1) \qquad -E_o[h] + \sum h(k|\ell)\gamma(k|\ell) \geq 0$$

for all h where we have set $\lambda = 1$ and:

$$(C.2) \qquad E_o[h] = \text{Min}\langle \sum h(k|\ell)a_k^+ a_\ell \rangle$$

If we choose a representation in which a given h is diagonal; that is:

$$(C.3) \qquad \sum h(k|\ell)a_k^+ a_\ell = \sum \varepsilon_k a_k^+ a_k$$

then $E_o[h]$ is quite easy to evaluate. It is given by:

$$(C.4) \qquad E = -\sum_{(-)} |\varepsilon_k|$$

where the sum is over the negative energy states of h. Then equation (C.1) is:

$$(C.5) \qquad \sum_{(-)} |\varepsilon_k|(1-\gamma(k|k)) + \sum_{(+)} \varepsilon_k \gamma(k|k) \geq 0 \ .$$

But this is immediately satisfied if:

$$0 \leq \gamma(k|k) \leq 1 \qquad \text{Q.E.D.}$$

Appendix D

We want to obtain a bound on the value of:

$$(D.1) \qquad \Lambda = \sum F^*(1,1')\Gamma(1,1'|2,2')F(2,2')$$

$$(D.2) \qquad \text{where:} \quad F(1,2) = -F(2,1)$$

$$(D.3) \qquad \text{and:} \quad \sum |F(1,2)|^2 = 1$$

We shall assume that both F and Γ are real. If we consider F as a matrix then by (D.2) the associated matrix, iF, is hermitian and may therefore be written in an eigenfunction expansion, with real eigenvalues. Hence:

$$(D.4) \qquad F(1,2) = -i \sum_n \lambda_n f_n(1) f_n^*(2).$$

Then:

$$(D.5) \qquad \Lambda = \sum_{\substack{n,m,1,1',\\ 2,2'}} \lambda_n \lambda_m f_n^*(1) f_n(1') \Gamma(1,1'|2,2') f_m(2) f_m^*(2')$$

If we construct the matrix:

$$(D.6) \qquad \tilde{\Gamma}_{nm} = \sum f_n^*(1) f_n(1') \Gamma(1,1'|2,2') f_m(2) f_m^*(2')$$

then it is not difficult to show, using the non-negativity of Γ that Γ is a non-negative matrix.

$$(D.7) \qquad \text{Then:} \quad \Lambda = \sum_{n,m} \lambda_n \tilde{\Gamma}_{nm} \lambda_m.$$

Since: $\sum \lambda_n^2 = 1$, it is clear that:

$\Lambda \leq$ Max. eigenvalue of $\tilde{\Gamma}$. But for a non-negative matrix the maximum eigenvalue can never exceed the trace thus we have the inequality:

$$\Lambda \leq \sum_n \tilde{\Gamma}_{nn} \tag{D.8}$$

In order to now obtain a bound on Λ we make use of the fact that since $G^{(1)}$ is a non-negative operator:

$$\sum_{\substack{1,1' \\ 2,2'}} f_n(1) f_n(1') (\delta_{12}\gamma(1'|2') - \Gamma(2,1'|1,2')) f_n^*(2) f_n^*(2') \geq 0 \tag{D.9}$$

Using the fact that:

$$\sum f_n(1)\delta_{12} f_n^*(2) = 1 \tag{D.10}$$

equation (D.9) becomes:

$$(f_n, \gamma f_n) \geq \tilde{\Gamma}_{nn} \tag{D.11}$$

We therefore obtain our result:

$$\Lambda \leq \sum_n \tilde{\Gamma}_{nn} \leq \sum (f_n, \gamma f_n) \leq N \ . \tag{D.12}$$

Appendix E

We shall first prove our conjecture for a 2 x 2 matrix. Given a matrix:

$$\begin{bmatrix} a_1 & b \\ b & a_2 \end{bmatrix}$$

(E.1) where: $a_1 \geq 0$, $a_2 \geq 0$, $b \geq 0$,

(E.2) and: $a_1 a_2 - b^2 \geq 0$,

we may write it as the sum of two matrices as follows:

$$(E.3) \quad \begin{bmatrix} a_1 & b \\ b & a_2 \end{bmatrix} = \begin{bmatrix} a_1 & b \\ b & b^2/a_1 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & C \end{bmatrix}$$

But according to (E.2) the constant C is non-negative. The reader may verify that the two matrices on the right hand side are in fact both positive constants times projection operators for vectors with non-negative elements.

The case of 3 x 3 matrices is somewhat more complicated. Suppose we are given a matrix of the following form, all of whose elements are non-negative:

$$(E.4) \quad M = \begin{bmatrix} a_1 & b_1 & b_3 \\ b_1 & a_2 & b_2 \\ b_3 & b_2 & a_3 \end{bmatrix} .$$

If the matrix is non-negative then the following determinantal

inequalities hold:

(E.5) $\det M \geq 0$

(E.6) $a_1 a_2 \geq b_1^2$

(E.7) $a_1 a_3 \geq b_3^2$

(E.8) $a_2 a_3 \geq b_2^2$.

Multiplying the last three inequalities in pairs we obtain

(E.9) $$a_1 a_2 \geq \frac{b_2^2 b_3^2}{a_3^2}$$

(E.10) $$a_1 a_3 \geq \frac{b_1^2 b_2^2}{a_2^2}$$

(E.11) $$a_2 a_3 \geq \frac{b_1^2 b_3^2}{a_1^2}$$.

We shall now show that not all of the right hand sides of the last three inequalities can be larger than the right hand side of the corresponding inequality above them. Assume:

(E.12) $$b_1^2 \leq \frac{b_2^2 b_3^2}{a_3^2}$$

(E.13) and: $$b_3^2 \leq \frac{b_1^2 b_2^2}{a_2^2}$$.

Then:

(E.14) $$b_1^2 b_3^2 \leq \left(\frac{b_1^2}{a_1 a_2}\right)\left(\frac{b_2^2}{a_2 a_3}\right)\left(\frac{b_3^2}{a_1 a_3}\right) \quad b_2^2 a_1^2 \quad .$$

By substituting unity for the expressions in brackets above we can only increase the inequality since each expression is less than or equal to one. Hence

(E.15) $$\frac{b_1^2 b_3^2}{a_1^2} \leq b_2^2 \quad .$$

Thus we may always assume that at least one of the three possible inequalities of the form (E.15) holds. Without loss in generality let us assume it is in fact (E.15). Then we may write the matrix M as:

(E.16) $$M = \begin{bmatrix} a_1 & b_1 & b_3 \\ b_1 & b_1^2/a_1 & b_1 b_3/a_1 \\ b_3 & b_1 b_3/a_1 & b_3^2/a_1 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & C_1 & d \\ 0 & d & C_2 \end{bmatrix}$$

where C_1, C_2, and d are all non-negative. In order to reduce our problem to the previous one of 2 x 2 matrices we need only show that the second matrix is non-negative. That is that:

(E.17) $$C_1 C_2 - d^2 \geq 0 \ .$$

(E.18) But: $$C_1 = a_2 - b_1^2/a_1 \ ,$$

(E.19) $$C_2 = a_3 - b_3^2/a_1 \ ,$$

(E.20) and: $$d = b_2 - b_1 b_3/a_1 \ ,$$

(E.21) Hence: $C_1 C_2 - d^2 = \frac{1}{a_1} \det M \geq 0.$

Since the first matrix of (E.16) is a projection operator for the unnormalized vector $(\sqrt{a_1}\ ,\ b_1/\sqrt{a_1}\ ,\ b_3/\sqrt{a_1})$ we have accomplished our reduction to the 2 x 2 case.

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